

ABSTRACT

5 The present invention relates to a data storage
medium encoded with the corresponding structure
coordinates of molecules and molecular complexes which
comprise the active site binding pockets of JNK3. A
computer comprising such data storage material is capable
10 of displaying such molecules and molecular complexes, or
their structural homologues, as a graphical three-
dimensional representation on a computer screen. This
invention also relates to methods of using the structure
coordinates to solve the structure of homologous proteins
15 or protein complexes. In addition, this invention
relates to methods of using the structure coordinates to
screen and design compounds, including inhibitory
compounds, that bind to JNK3 or homologues thereof. This
invention also relates to molecules and molecular
20 complexes which comprise the active site binding pockets
of JNK3 or close structural homologues of the active site
binding pockets.